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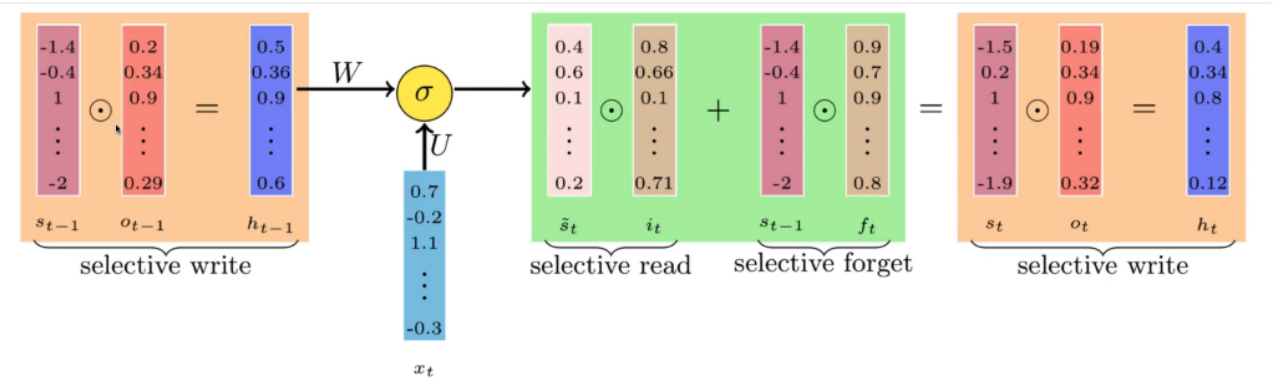
How LSTMs solve the problem of Vanishing Gradients?

Parveen Khurana Jul 21, 2019 · 13 min read

This article covers the content discussed in the Vanishing and Exploding Gradients and LSTMs module of the Deep Learning course offered on the website: https://padhai.onefourthlabs.in

We discussed in case of RNNs that while back-propagating, gradients might vanish or gradients might explode as discussed in this article and so from there, we move on to the concepts of LSTMs and GRUs(discussed in this article) which uses selective read, write and forget to pass on the relevant information to the state vector.



LSTM Architecture

The gates regulate/control the flow of the information in LSTMs.

Gates:

$$o_t = \sigma(W_o h_{t-1} + U_o x_t + b_o)$$
$$i_t = \sigma(W_i h_{t-1} + U_i x_t + b_i)$$
$$f_t = \sigma(W_f h_{t-1} + U_f x_t + b_f)$$

States:

$$\tilde{s}_t = \sigma(W h_{t-1} + U x_t + b)$$
$$s_t = f_t \odot s_{t-1} + i_t \odot \tilde{s}_t$$
$$h_t = o_t \odot \sigma(s_t)$$

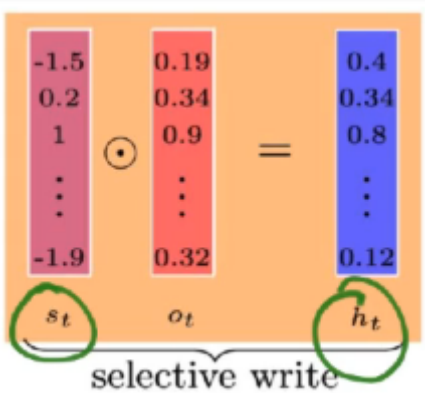
Gates and the corresponding state used in the LSTM

Intuition: How gates help to solve the problem of vanishing gradients

During forward propagation, gates control the flow of the information. They prevent any irrelevant information from being written to the state.

Similarly, during backward propagation, they control the flow of the gradients. It is easy to see that during the backward pass, gradients will get multiplied by the gate.

Let's consider the following output gate:



We can write the hidden state **ht** as:

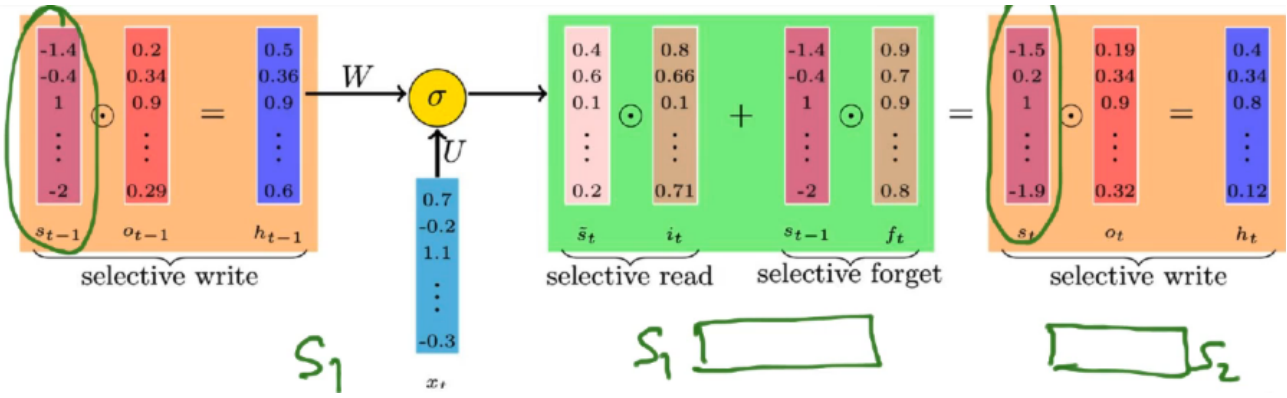
ht = (st)*(ot) (Equation 1)

Now let's say we wish to compute the derivative of the Loss function with respect to **W**, now in that derivative, at some point we would encounter the derivative of this (**ht**) with respect to (**st**) (as we would be back-propagating and **ht** is derived as the multiplication of **st** with some numbers(**st** is multiplied with the **ot** gate)). And this

derivative of (**ht**) with respect to (**st**) would just be (**ot**) as is clear from **equation 1**. So, that means somewhere in the chain of derivative, (while computing the derivative of the Loss function with respect to W) we would have multiplication with this (**ot**).

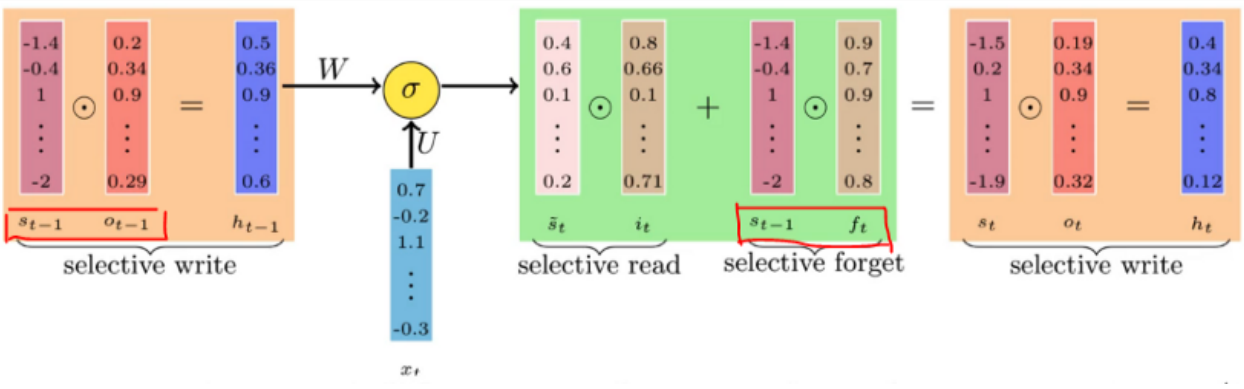
And the same would be there for the other gates as well; somewhere in the chain of the derivative, these gates would be there.

Just as in the forward propagation, things are being multiplied by gates and these gates decides in a way how much of information it needs to pass, during backward propagation also, the gradients are getting multiplied by gates and these gates control the backward flow of information because this gradient is deciding how much of this gradient needs to flow back.



Let say we write **s(t-1)** as **s1** and **st** as **s2**(that is '**t**' is 2 in this case).

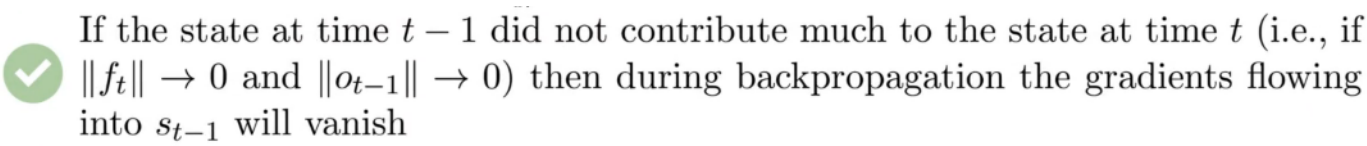
If we say that **s1** did not contribute much to the state **s2** that means the value of the output gate(**o(t-1)**) and the forget gate(**ft**) would be close to 0 as these two gates are used with **s(t-1)**(**s1** in this case) as shown in the image below(highlighted in red box in the below image):



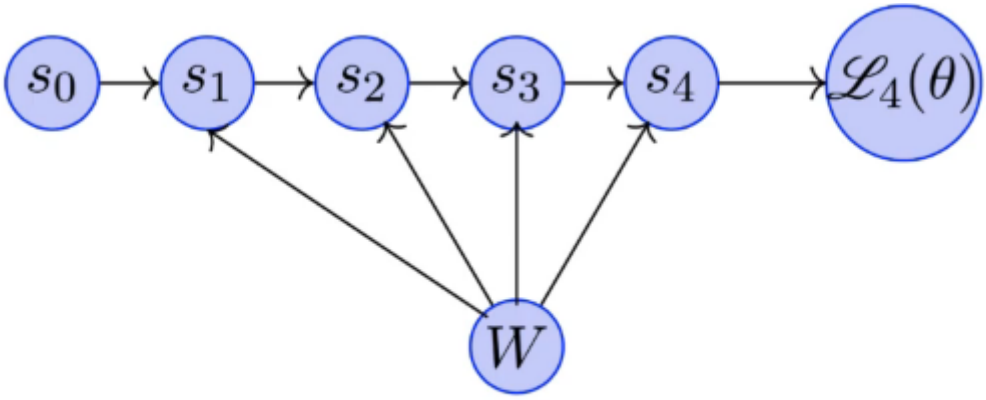
So, if both the gates i.e the output gate **o(t-1)** and the forget gate **ft** are close to 0, then we can say that **s(t-1)**(**s1** in this case) did not contribute much to **st**(**s2** in this case).

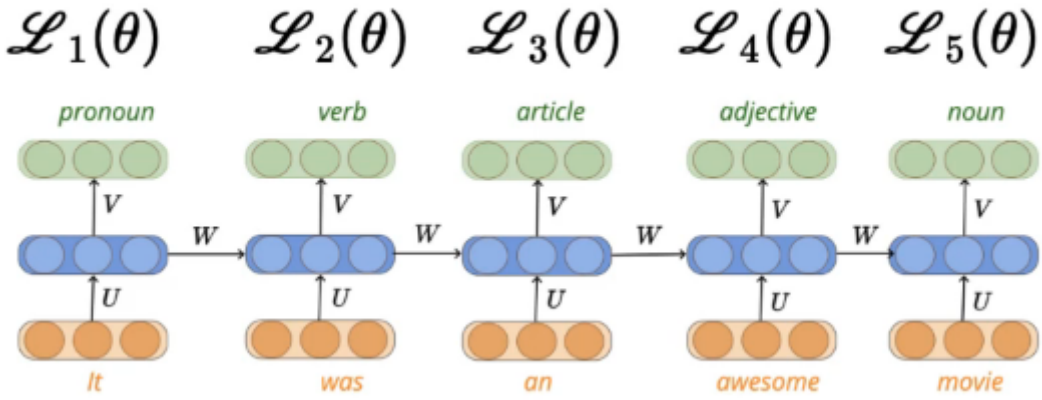
Now what would happen in this case during backpropagation is that, we would again have these gates **ft** and **o(t-1)** because that would show up somewhere in the chain rule, and since these two quantities(**ft** and **o(t-1)**) are close to 0, the overall gradient would go to 0 and we would have a vanishing gradient problem.

The key difference from the vanilla RNN is that the flow of information and the gradients both are controlled by the gates; what this means is that since in this case, we have both **ft** and **s(t-1)** close to 0, that means during the forward pass itself, **s1** did not contribute anything to **s2**, so holding **s1** responsible for errors in the Loss function does not make sense as the **s1** information was blocked by these gates and it did not carry on forward hence the gradients did not flow back. So, this synchronous thing that **whatever happens in the forward pass also happens in the backwards pass; because the gates did not allow the information to flow forward hence the information is not flowing backward**, this kind of vanishing problem is okay, it does not the effect the model, **if we did not contribute in the forward pass then we don't need any feedback in the backward pass**.

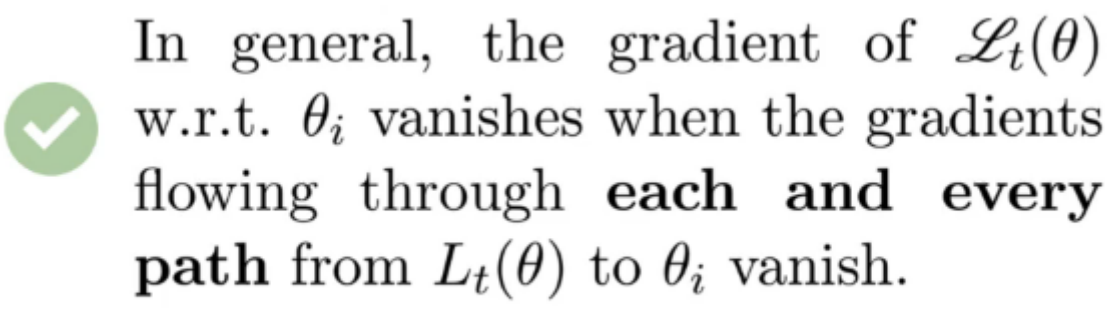


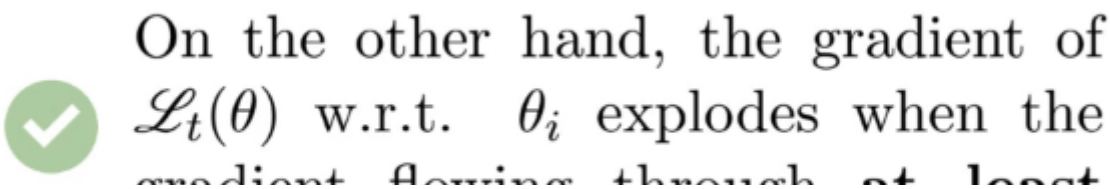
Revisiting RNNs:





Let's say we want to compute the **gradient** of the **Loss function** with respect to **W**, so it would be **summation of derivative of loss function** with respect to **W** over all possible paths as discussed in previous articles, and since this summation over all the paths is there, for the overall gradient to vanish, gradients along all these paths must vanish and the overall gradient would explode if gradient along any one of the path explodes.





gradient flowing through at least **one path** explodes.

theta_i refers to one of the weight

Dependency Diagram for LSTMs

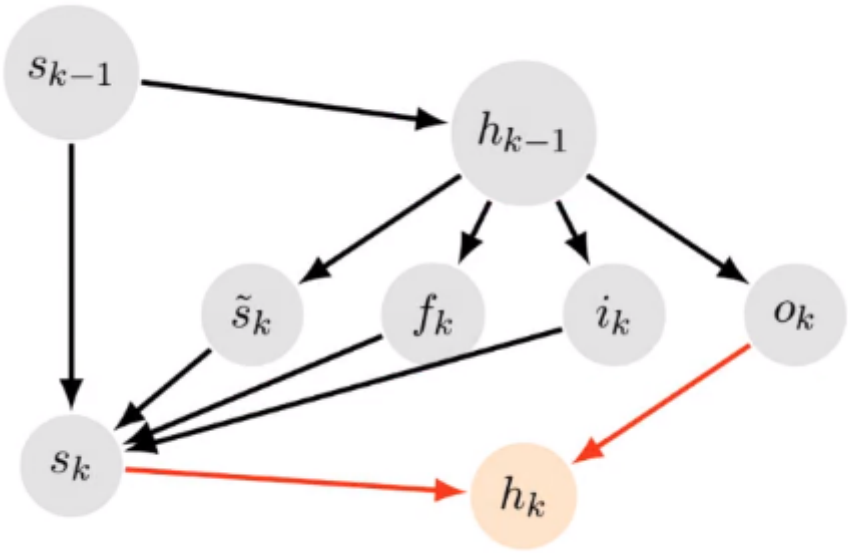
The equations involved in the LSTM are as follows:

$$o_k = \sigma(W_o h_{k-1} + U_o x_k + b_o)$$
$$i_k = \sigma(W_i h_{k-1} + U_i x_k + b_i)$$
$$f_k = \sigma(W_f h_{k-1} + U_f x_k + b_f)$$
$$\tilde{s_k} = \sigma(W h_{k-1} + U x_k + b)$$
$$s_k = f_k \odot s_{k-1} + i_k \odot \tilde{s_k}$$
$$h_k = o_k \odot \sigma(s_k)$$

First 3 equations are of the gates used in LSTMs, then the next 3 equations represent the states that we compute and last two equations(for sk and hk) compute/represent the output for the LSTM

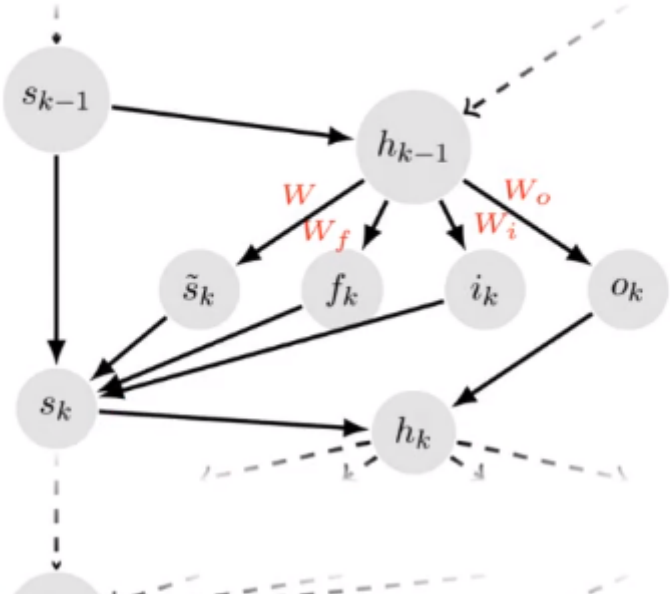
$$o_k = \sigma(W_o h_{k-1} + U_o x_k + b_o)$$
$$i_k = \sigma(W_i h_{k-1} + U_i x_k + b_i)$$
$$f_k = \sigma(W_f h_{k-1} + U_f x_k + b_f)$$
$$\tilde{s_k} = \sigma(W h_{k-1} + U x_k + b)$$
$$s_k = f_k \odot s_{k-1} + i_k \odot \tilde{s_k}$$
$$h_k = o_k \odot \sigma(s_k)$$

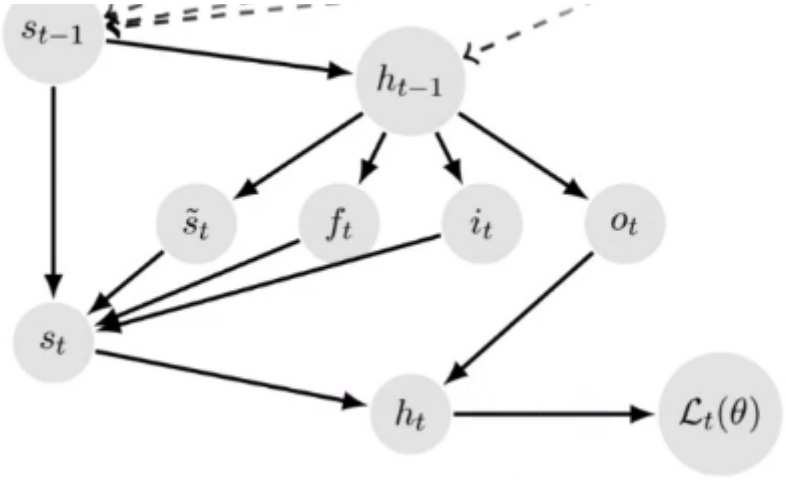
We have two inputs here(in the above equations), **h(k-1)** and **s(k-1)** to compute the new state **sk** and **hk**, **sk(~)** is just an intermediate input(temporary state) and not an actual input and is computed from **h(k-1)**. **xk** is also there but we are not going to consider it here just like in the case of dependency diagram of RNN where we don't consider the input x and show all the computations in the terms of state only.



This is the dependency diagram to go from one state(s(k-1), h(k-1)) to another state(sk, hk in this case) in case of LSTM.

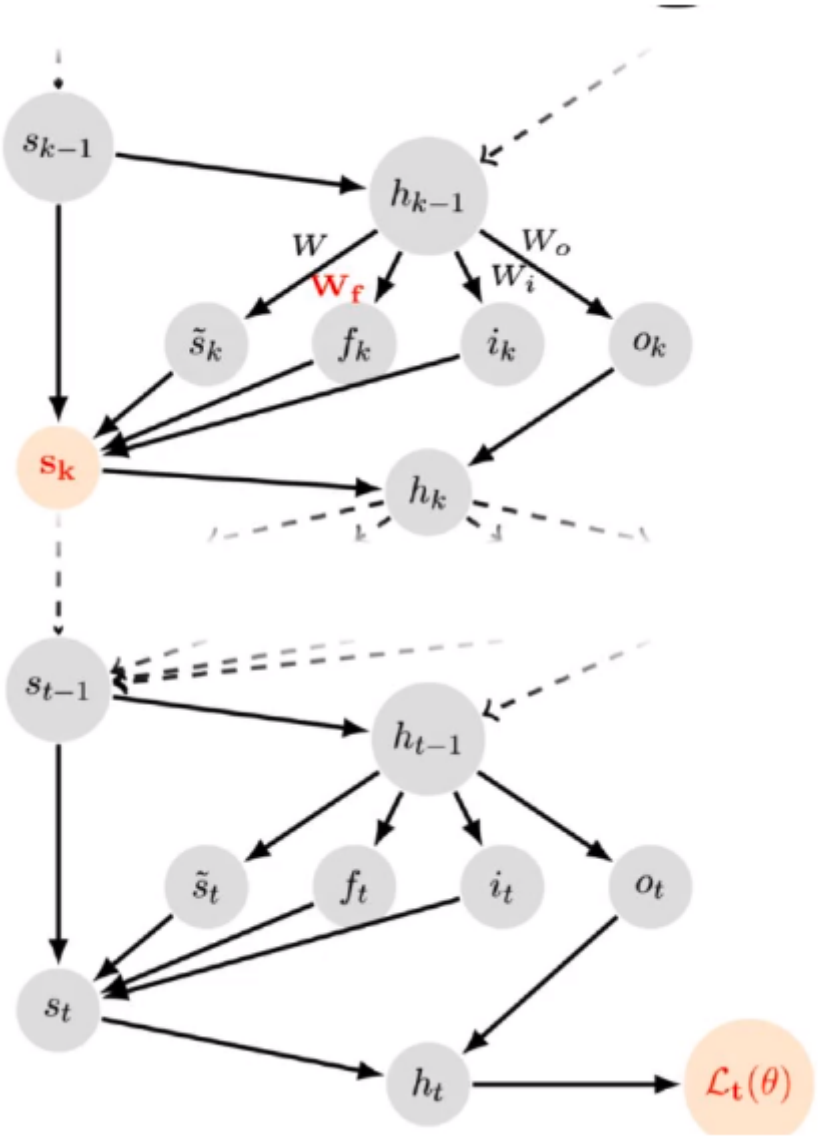
The same thing is going to repeat at subsequent time steps also meaning that the dependency diagram for a particular time step looks exactly the same as that at some other time step with the only change being in the subscript of the state vector i.e at **1st time step** it would be **s1**, **h1**; at **2nd time step** it would be **s2**, **h2** and so on.





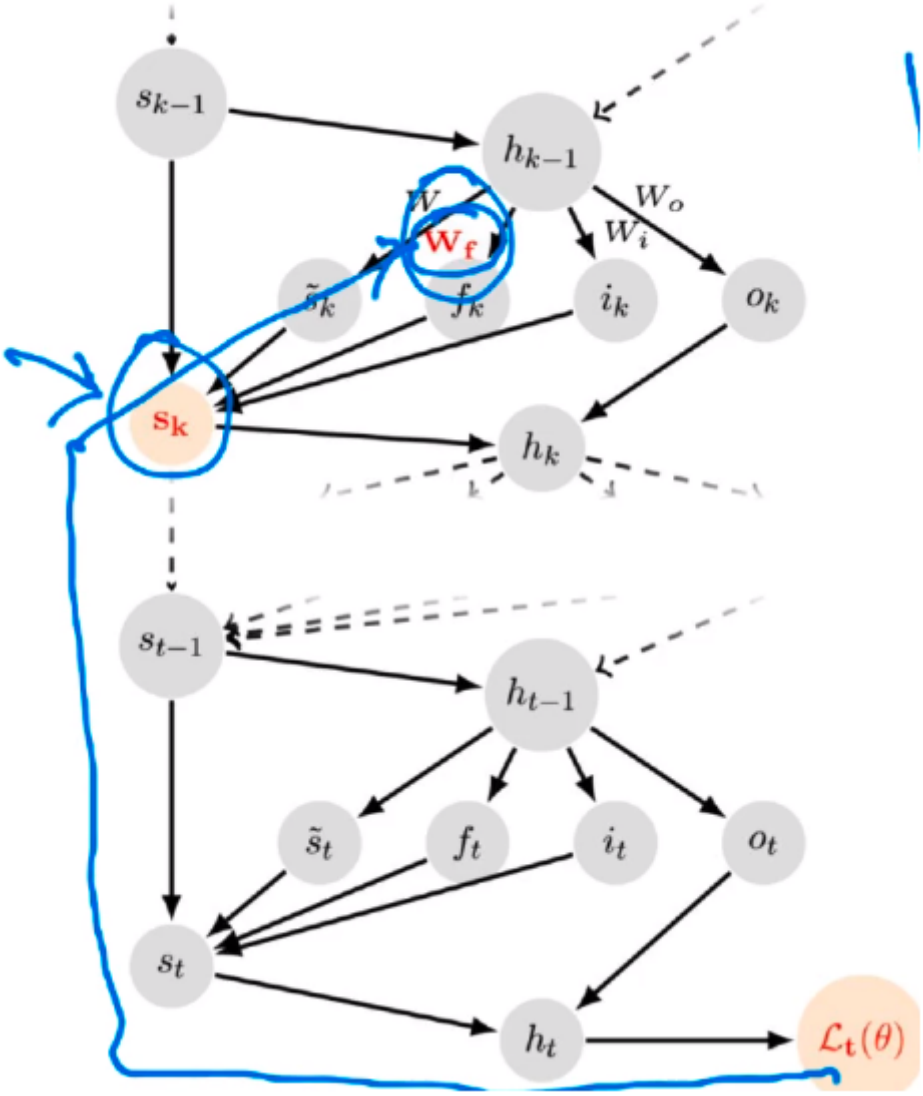
ht represents the final state at time step t from which we compute the Loss value.

We will focus on one of the weight and the same argument will hold for other weights also. Let's consider weight Wf(in red in the below image).



We are interested in knowing if the gradient flows to **Wf** through **sk**(we are considering the scenario just like in case of RNNs i.e if **Wf** was wrong hence **sk** was

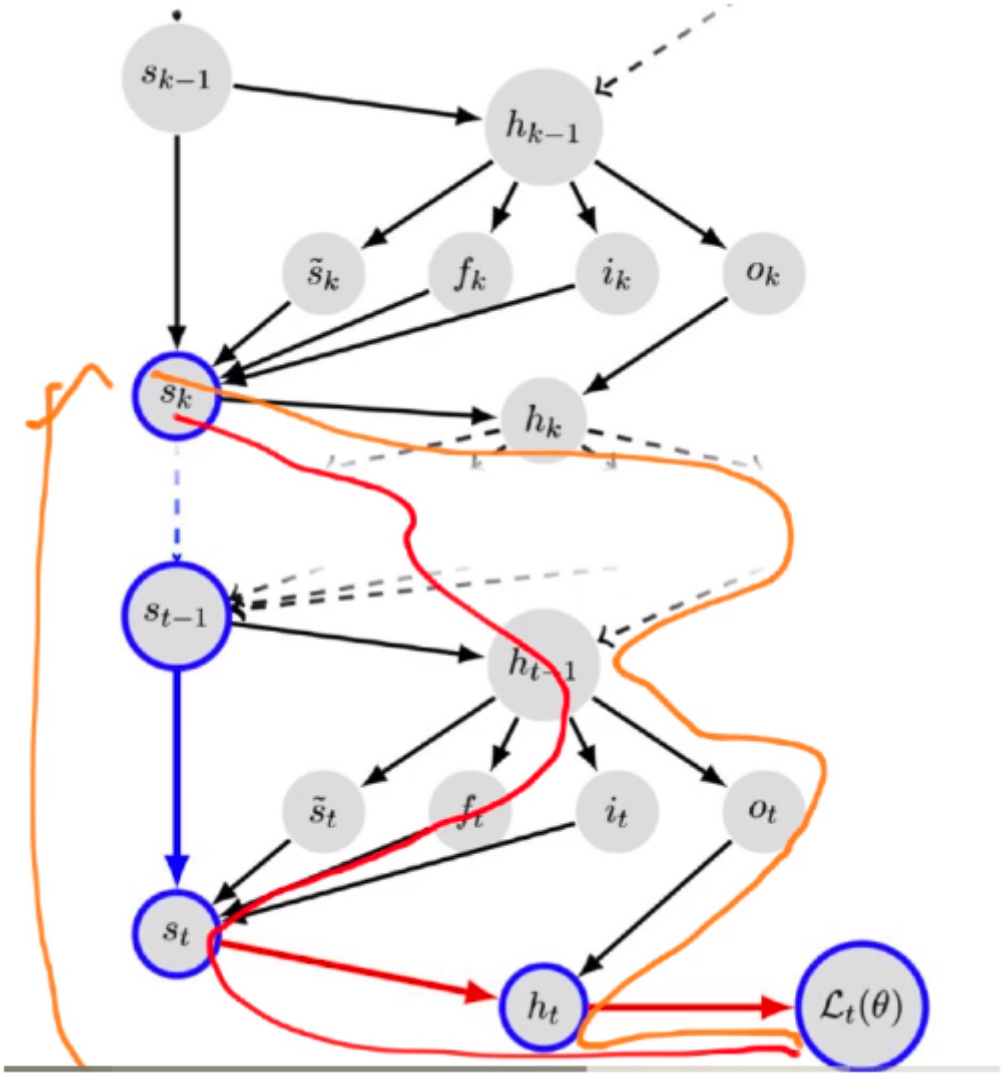
wrong and hence the loss was high then we need to pass this information back to **Wf** through **sk**).



It is enough to show that the gradient flows up to **sk** because from **sk**, **Wf** is very nearby(from **sk**) and if the gradient flows up to **sk** then it's okay. To reach up to **sk**, multiple time steps are there and from **sk** to **Wf** only two more steps are there so we need to just ensure that gradient flows up to **sk**.

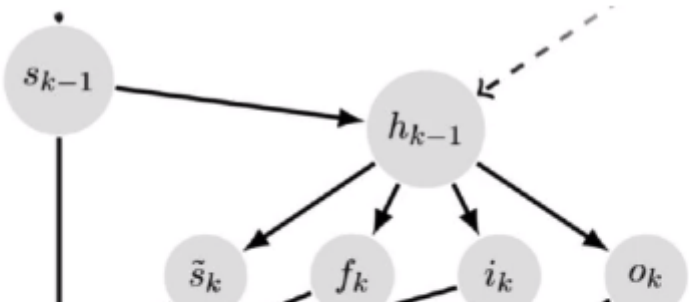
It is sufficient to show that $\frac{\partial \mathcal{L}_t(\theta)}{\partial s_k}$ does not vanish (because if this does not vanish we can reach W_f through s_k

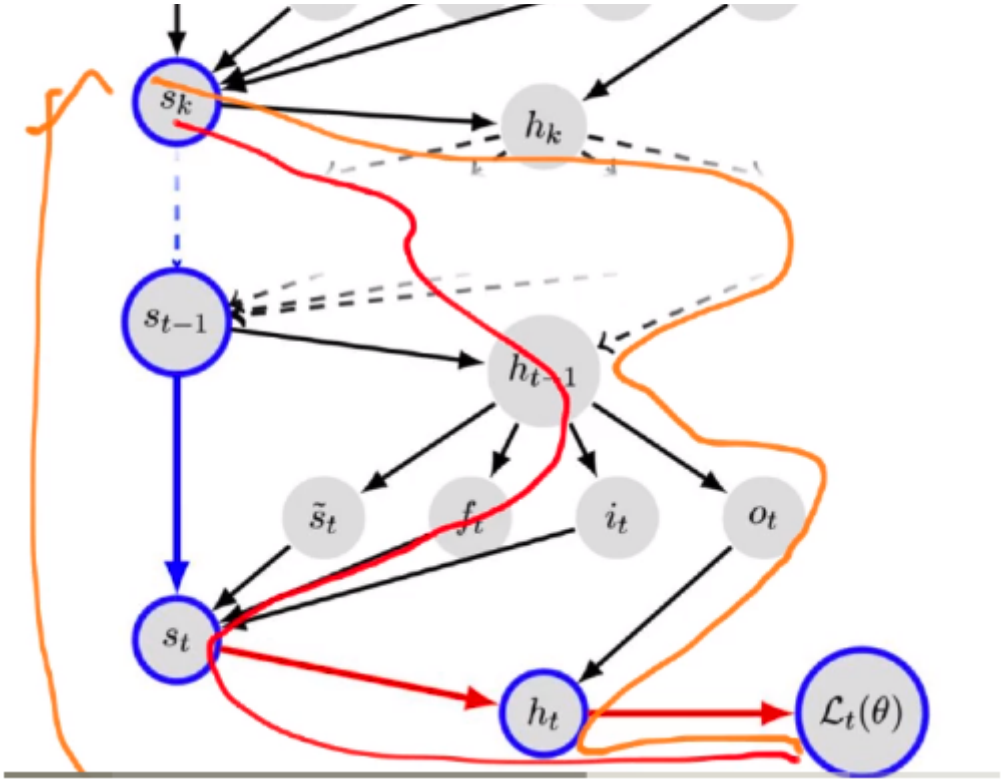
Now from **L(theta)** to **sk**, we have multiple paths and for the case of vanishing gradients, we need to show that the gradient does not vanish along any one of these paths.



As there are multiple paths, the overall gradient of **L(theta)** with respect to **sk** is going to be the sum of derivative across all these paths. And now to show that the overall gradient does not vanish, it would be sufficient to show that gradient does not vanish across one of these paths.

So, we have taken one such path(highlighted in blue nodes in the below image) and let's say we call the gradient across that path as **t0**. So, this **t0** would look like:





$$t_0 = \frac{\partial \mathcal{L}_t(\theta)}{\partial h_t} \frac{\partial h_t}{\partial s_t} \frac{\partial s_t}{\partial s_{t-1}} \cdots \frac{\partial s_{k+1}}{\partial s_k}$$

We will not bother much about the highlighted part(in the image below) as this is directly connected to **ht** and along a single path the gradient may not vanish so that's okay for us. The derivative of **ht** with respect to **st** would also be okay, our main concern is with the part in the blue in the image below as that part would again be a multiplication of multiple terms.

$$t_0 = \frac{\partial \mathcal{L}_t(\theta)}{\partial h_t} \boxed{\frac{\partial h_t}{\partial s_t}} \frac{\partial s_t}{\partial s_{t-1}} \cdots \frac{\partial s_{k+1}}{\partial s_k}$$

We have **ht** as the following:

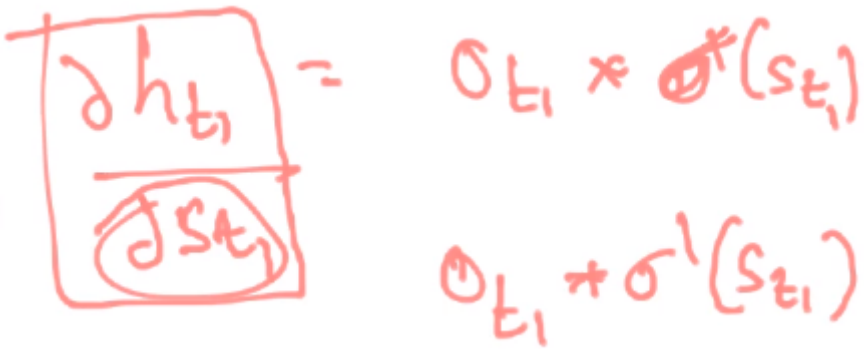
$$h_t = o_t \odot \sigma(s_t)$$

So, **ht** is given the output gate multiplied with the **sigmoid** over **st**

Every element of **ht** depends only on one element of **ot** and one element of **st**, so we would have:

ht1 = (ot1)*(sigmoid of st1)

Now **ht** is a '**d**' dimensional vector and **st** is also a '**d**' dimensional vector, so the derivative of **ht** with respect to **st** is going to be a '**d X d' dimensional matrix** with all the off-diagonal elements as 0(as discussed in the Vanishing and Exploding Gradients article: https://medium.com/@prvnk10/vanishing-and-exploding-gradients-52af750ede32). So, this matrix would be a diagonal matrix. The first element of this matrix would be:



So, we can write the derivative of ht with respect to st as:

$$\frac{\partial h_t}{\partial s_t} = \mathcal{D}(o_t \odot \sigma'(s_t))$$

Here, D means it is a Diagonal matrix with diagonal elements as the Hadamard product of ot with the derivative of sigmoid of corresponding st value.

Now we want to compute the next term in the equation of t0.

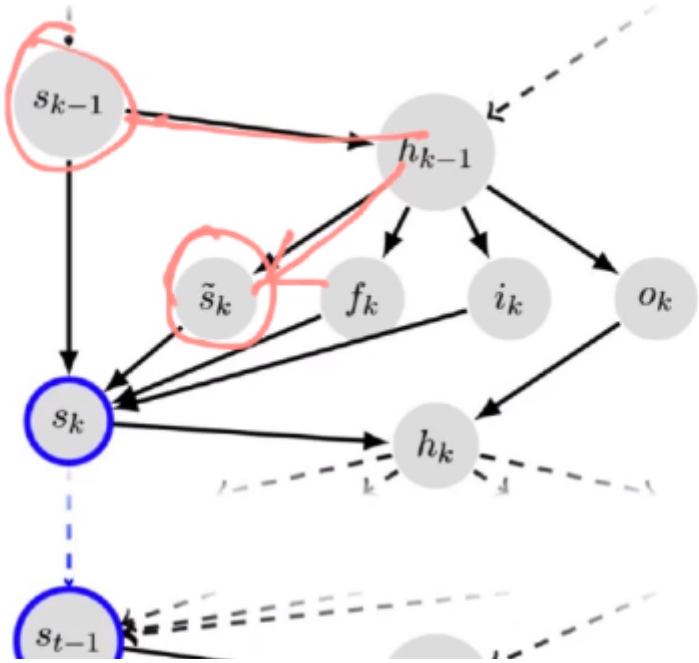
$$t_0 = \frac{\partial \mathcal{L}_t(\theta)}{\partial h_t} \frac{\partial h_t}{\partial s_t} \boxed{\frac{\partial s_t}{\partial s_{t-1}}} \cdots \frac{\partial s_{k+1}}{\partial s_k}$$

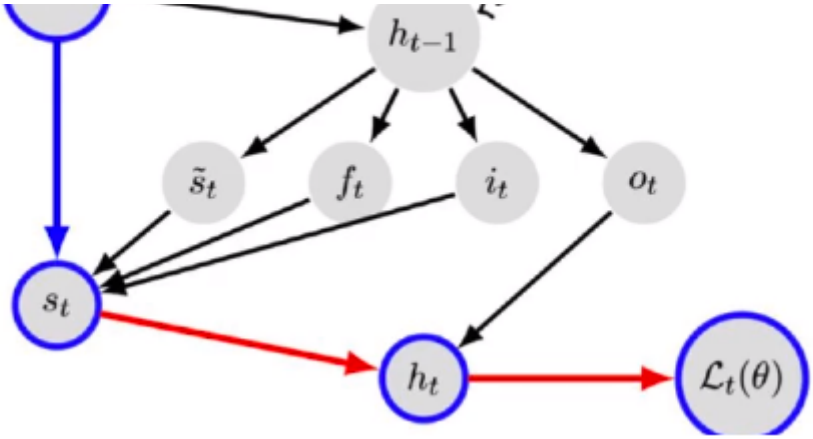
So, we consider the derivative of **st** with respect to **s(t-1)**.

We have **st** as the following:

$$s_t = f_t \odot s_{t-1} + i_t \odot \tilde{s}_t$$

Now this **st(~)** also depends on **s(t-1)** as is clear in the below image

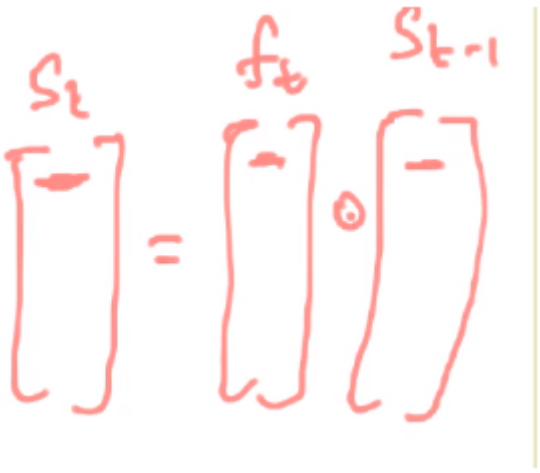




The derivative of **st** with respect to **s(t-1)** is going to be the sum of the derivative of two terms(as in the formula of the **st**) with respect of **s(t-1)** and our goal is show that the overall gradient does not vanish. So, we make an assumption that let's say derivative of **st(~)** with respect to **s(t-1)** actually vanishes and we show that the derivative of the first term(i.e (**ft** * **s(t-1)**)) with respect to **s(t-1)** does not vanish then our work would be done as some value would be there which would imply that the gradient does not vanish. So, we only focus on the first quantity(highlighted in the below image).

$$s_t = f_t \odot s_{t-1} + i_t \odot \tilde{s}_t$$

Now we have st as:



So, we can say that every element of **st** depends on only one element of **ft** and one element of **s(t-1)**. And **st** is a '**d**' dimensional vector and **s(t-1)** is also a '**d**' dimensional

vector, so the derivative of **st** with respect to **s(t-1)** would be a matrix with dimensions '**dX d**' and with off-diagonal elements as 0.

$$\frac{\partial s_t}{\partial s_{t-1}} = \mathcal{D}(f_t)$$

Similarly, we can write the derivative of state at some other time step as well with respect to the previous state as a diagonal matrix with off-diagonal elements as 0 and the diagonal elements as the value of the forget gate at the corresponding index.

So, the overall term t0 looks as:

$$\begin{aligned} t_0 &= \frac{\partial \mathcal{L}_t(\theta)}{\partial h_t}\frac{\partial h_t}{\partial s_t}\frac{\partial s_t}{\partial s_{t-1}}\cdots\frac{\partial s_{k+1}}{\partial s_k} \\ &= \mathcal{L}_t'(h_t).\mathcal{D}(o_t \odot \sigma'(s_t))\mathcal{D}(f_t)\ldots\mathcal{D}(f_{k+1}) \end{aligned}$$

Now if we have the multiplication of multiple diagonal matrices, we can write the resultant as a single diagonal matrix with corresponding elements of all the matrices being multiplied. Example:

$$\begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}\begin{bmatrix} c & 0 \\ 0 & d \end{bmatrix}\begin{bmatrix} e & 0 \\ 0 & f \end{bmatrix} = \begin{bmatrix} ace & 0 \\ 0 & bdf \end{bmatrix}$$

If we multiply many diagonal matrices then the product is a product of all the corresponding diagonal elements(so we get a matrix whose elements is the product of all the corresponding diagonal elements)

$$t_0 = \frac{\partial \mathcal{L}_t(\theta)}{\partial h_t}\frac{\partial h_t}{\partial s_t}\frac{\partial s_t}{\partial s_{t-1}}\cdots\frac{\partial s_{k+1}}{\partial s_k}$$

$$= \mathcal{L}'_t(h_t).\mathcal{D}(o_t \odot \sigma'(s_t))\mathcal{D}(f_t)\dots\mathcal{D}(f_{k+1})$$
$$= \mathcal{L}'_t(h_t).\mathcal{D}(o_t \odot \sigma'(s_t))\mathcal{D}(f_t \odot \dots \odot f_{k+1})$$
$$= \mathcal{L}'_t(h_t).\mathcal{D}(o_t \odot \sigma'(s_t))\mathcal{D}(\odot_{i=k+1}^{t} f_i)$$

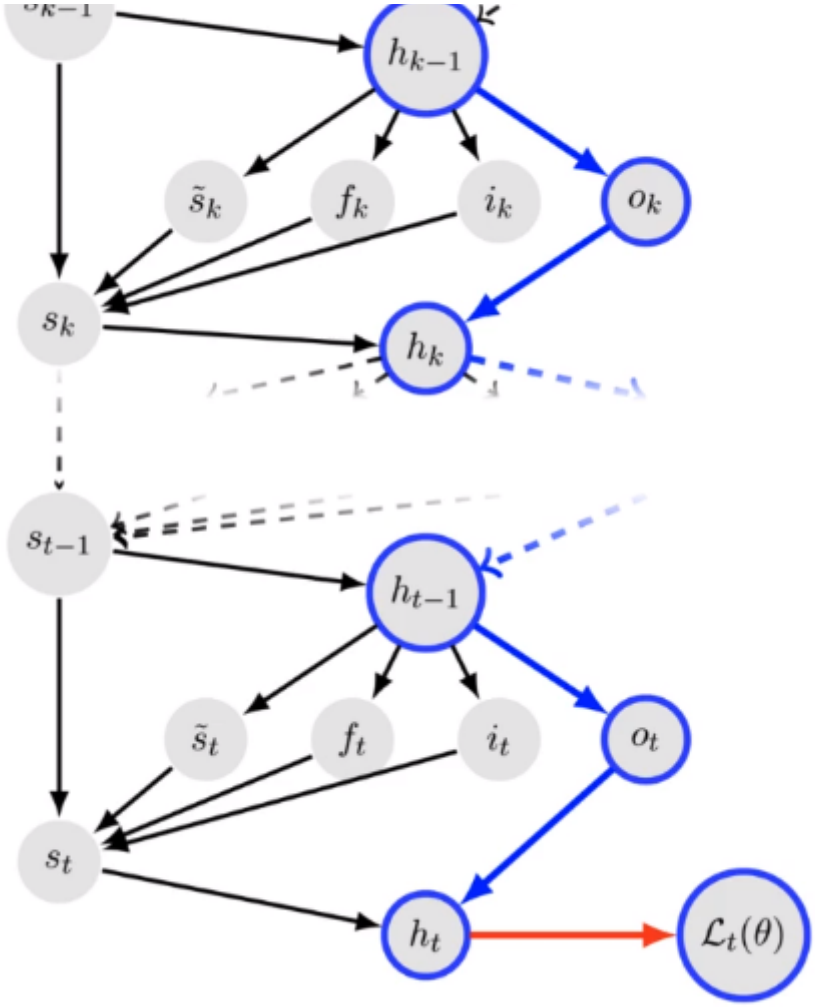
In the last equation, we have written the single diagonal matrix(in blue) as the product of all the forget gates from time step k+1 to time step t.

Now the gradients would vanish if all the forget gates i.e **f1, f2, f3**, ….., all the way up to the last forget gate **ft** are very very small, then, in that case, the entire gradient would vanish so it looks like the gradients could still vanish but the catch here is that if **f1** was very small that means **s1** did not contribute much to s2(as explained in the start of this article); if **f2** is small it means **s2** did not contribute much to **s3**; in turn what it means is that **s1** anyways did not contribute much to **s2**, **s2** has also not contributed much to **s3** that means **s1** did not contribute almost anything to **s3**, it contributed even less; now if **f4** is also small that means **s3** did not contribute anything to **s4** and hence the same argument that **s1** is contributing even less to **s4** so based on this we can say that the contribution has vanished by the time we have reached **s4** because the gates were very small; in the same way in the backward direction the gradients from **s4** will vanish by the time we reach **s1** but this kind of vanishing is not a problem because if in the forward direction it did not contribute that in the backward if the gradients do not reach to that state that is okay as no feedback is required in the backward time when the state did not contribute in the forward pass. So, the gates control the flow of information in both directions.

Dealing with exploding gradients:

For the overall gradient to explode, we need to show the gradient explodes at least along one of the paths and that would be sufficient to say that the overall gradient explodes.

So, we are considering the derivative of the Loss function with respect to **s(k-1)** (one of the terms that appear in the chain rule) and we have considered one of the possible paths(in blue nodes in the below image) that lead from **Loss value(L) to s(k-1)**



The derivative as per the chain rule would look like:

$$t_1 = \frac{\partial \mathcal{L}_t(\theta)}{\partial h_t} \left(\frac{\partial h_t}{\partial o_t} \frac{\partial o_t}{\partial h_{t-1}} \right) \cdots \left(\frac{\partial h_k}{\partial o_k} \frac{\partial o_k}{\partial h_{k-1}} \right)$$

The term in blue parentheses(above image)(**3 nodes ht, ot, h(t-1)**) would keep repeating all the way back.

Now the derivative of **ht** with respect to **ot** is going to a be diagonal matrix as discussed in the case of vanishing gradients(that the derivative of a '**d**' dimensional vector with respect to a '**d**' dimensional vector is going to be a '**d X d**' dimensional matrix).

We have **ot**(represented as **ok** for **k'th time step**) as the following:

$$o_k = \sigma(W_o h_{k-1} + U_o x_k + b_o)$$

Let's ignore the sigmoid for a moment(anyways it's just going to add one more term in the chain nothing more than that), then the last two terms in the above equation are constant and the derivative of **ok** with respect to **h(k-1)** would simply be **Wo**.

So, we can write the derivative as:

$$
\begin{aligned}
t_1 =& \frac{\partial \mathcal{L}_t(\theta)}{\partial h_t} \left(\frac{\partial h_t}{\partial o_t} \frac{\partial o_t}{\partial h_{t-1}} \right) \dots \left(\frac{\partial h_k}{\partial o_k} \frac{\partial o_k}{\partial h_{k-1}} \right) \\
=& \mathcal{L}'_t(h_t) \left(\mathcal{D}(\sigma(s_t) \odot o'_t).W_o \right) \dots \\
& \left(\mathcal{D}(\sigma(s_k) \odot o'_k).W_o \right)
\end{aligned}
$$

All the individual terms in the blue parentheses would have one diagonal matrix and Wo

All the individual terms in the blue parentheses would have one diagonal matrix and Wo, so we expand it out(this is a matrix multiplication), so if we club all the diagonal matrices together we get one large diagonal matrix and **Wo** is getting multiplied as many times as the number of terms in the chain, we call the magnitude of this large matrix as **K**, so we have:

$$
\begin{aligned}
t_1 =& \frac{\partial \mathcal{L}_t(\theta)}{\partial h_t} \left(\frac{\partial h_t}{\partial o_t} \frac{\partial o_t}{\partial h_{t-1}} \right) \dots \left(\frac{\partial h_k}{\partial o_k} \frac{\partial o_k}{\partial h_{k-1}} \right) \\
=& \mathcal{L}'_t(h_t) \left(\mathcal{D}(\sigma(s_t) \odot o'_t).W_o \right) \dots \\
& \left(\mathcal{D}(\sigma(s_k) \odot o'_k).W_o \right) \\
\|t_1\| \leq& \|\mathcal{L}'_t(h_t)\| \left(\|K\| \|W_o\| \right)^{t-k+1}
\end{aligned}
$$

So, if the highlighted value in the below image is large then the gradients would explode. So, LSTMs actually could not solve the problem of exploding gradients, the overall gradient could still explode and in practice the way we deal with it is that a gradient has some magnitude and a direction, so we want to go in the direction of the gradient but not with large magnitude so we move in the direction of the gradient but with a small magnitude and the technique is termed as clipping. So, clipping just

rescales the gradient so it lies in a certain magnitude range and we can still use the direction of the gradient.

$$
\begin{aligned}
t_1 &= \frac{\partial \mathcal{L}_t(\theta)}{\partial h_t}\left(\frac{\partial h_t}{\partial o_t}\frac{\partial o_t}{\partial h_{t-1}}\right)\cdots\left(\frac{\partial h_k}{\partial o_k}\frac{\partial o_k}{\partial h_{k-1}}\right) \\
&= \mathcal{L}'_t(h_t)\left(\mathcal{D}(\sigma(s_t)\odot o'_t).W_o\right)\cdots \\
&\qquad \left(\mathcal{D}(\sigma(s_k)\odot o'_k).W_o\right) \\
\|t_1\| &\leq \|\mathcal{L}'_t(h_t)\|\left(\|K\|\|W_o\|\right)^{t-k+1}
\end{aligned}
$$

So, while backpropagating if the norm of the gradient exceeds a certain value, it is scaled to keep its norm within an acceptable threshold.

So, in essence, we can say that LSTMs does not have the problem of vanishing gradients(gradients could vanish in case of LSTMs but that would be the case when the information does not flow in the forward direction in the forward pass and that would be okay as discussed in this article).

LSTMs does not actually solve the problem of exploding gradients. Gradients could still explode and the way we deal is that we move in the direction of the Gradient to update the parameters but we move with a small magnitude.

All the images used in this article is taken from the content covered in the Vanishing and Exploding Gradients and LSTMs module of the Deep Learning Course on the site: padhai.onefourthlabs.in

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